Ultraacoustic, Volumetric and Optical Studies of Nucleic Acid Bases and Nucleosides in Different Aqueous Solutions

Synopsis

For The Registration of

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1. Introduction

Volumetric, ultraacoustic and optical properties provide valuable information regarding the thermodynamic behaviour of different solutes such as amino acids, proteins, peptides, drugs, nucleotides, carbohydrates and other biomolecules in aqueous or non-aqueous media. Understanding the effect of cosolute and their interaction with biologically important molecules is a subject of research interest. These interactions provide idea about the structure making and breaking properties of solutes and activity of bioactive molecule in biological systems.

The thermodynamic stability of any biopolymer conformation is the net result of several secondary or non-covalent interactions which may occur intra-molecularly or with the solvent. So the physiochemical characterization of binary and ternary solutions as a function of temperature and concentration is of immense interest in biological systems. Measurements of thermodynamic properties provide valuable insights into various aspects of (biomolecules + solvent + cosolute) interactions.

Thermophysical properties and solution behaviour of solutes are depending on different interactions in solutions. Molecular interaction study in liquids provides information regarding internal structure, molecular association, complex formation, internal pressure etc. Ultrasonic velocity, density, refractive index and derived thermodynamic properties give qualitative information about molecular interaction in solutions.

Solute-solute and solute-solvent interactions are measured by acoustic, volumetric and optical properties of amino acids, proteins, peptides, drugs, nucleic acid bases, nucleosides, nucleotides, carbohydrates and other biomolecule in aqueous or non-aqueous solutions has got great importance in many fields such as pharmaceutical, medicinal chemistry, industrial processes, biochemistry etc. Proteins, carbohydrates, fats, nucleotides, carbohydrates, vitamins, nucleic acid bases, nucleosides, nucleotides and minerals are playing an important role in performing normal functions of cells.

Nucleic acid bases, nucleosides and nucleotides are present in the DNA RNA. They helps the body to synthesize many enzymes necessary for cell functioning. It is also used as an allosteric regulator in the body. And they can be used for drug delivery. It is therefore interesting to observe the interaction between nucleosides, nucleic acid base, nucleotides and other bioactive molecules in aqueous cosolute solutions. Review of literature reveals

that the thermodynamic properties of DNA and RNA components have not yet been fully investigated.

2. Review of literature and development in the subject

The thermodynamic properties of nucleic acid bases, nucleosides and nucleotides etc. is carried out by numbers of researcher in recent years. Analysis of properties such as density, ultrasound velocity, and refractive index over wide range of temperature, composition and in aqueous solutions of different cosolutes nucleic acid bases, nucleosides and nucleotides is still lacking in the literature.

Thermophysical of aqueous solutions play crucial role in understanding the nature of molecular interactions solution. It is necessary to study the thermodynamic properties of aqueous solution of nucleic acid bases, nucleosides and nucleotides in order to comprehend the mechanisms of their actions in detail. Volumetric, acoustic and optical properties are important tools in studying the solution behaviors of solutes and reveal valuable information about solute-solute/solute–solvent interactions in solution. There are very limited number of works in the literature for the volumetric, acoustic and optical properties of nucleic acid bases, nucleosides and nucleotides and their interpretations in terms of nucleic acid bases/nucleosides/nucleotides + water and nucleic acid bases/nucleosides/nucleotides + water + co-solute interactions in solution.

The mechanism of action of nucleic acid bases/nucleosides/nucleotides is quite complex and this needs knowledge about the molecular interactions in fluids. The data for acoustic, volumetric and optical properties on most of nucleic acid bases/nucleosides/nucleotides are quite being deficient in aqueous media and aqueous-cosolute solution. Therefore, we planned to carry out systematically the acoustic, volumetric and optical properties of nucleic acid bases/nucleosides/nucleotides in water and different cosolute media at different temperatures and atmospheric pressure.

The significant application of thermophysical parameters approach has very fruitful in the field of nucleic acid bases/nucleosides/nucleotides analysis in pure solvent and solvent mixtures. Hence, there is a need to widen this research in order to examine how the thermodynamic properties of various substances in solution incorporate in to nucleic acid bases/nucleosides/nucleotides to improve the activity biologically active compound in

solution. Based on the literature survey of acoustic, a volumetric and optical property of nucleic acid bases/nucleosides/nucleotides in water and different cosolute gives the essential thermodynamic properties so that they may improve the excellent activity of nucleic acid bases/nucleosides/nucleotides.

N. I. Nakano et al have investigated the molecular interactions of purines, and some other heteroatomic compounds in aqueous media. P.O. P. T'so has examined the interaction and association of bases and nucleosides in aqueous solutions. T.V. Chalikian has performed the volumetric properties of heterocyclic base and nucleosides in aqueous solution at different temperature. Thermodynamic analyses of nucleosides and nucleic acid bases in aqueous solutions at different temperature have performed by N. Kishore and S.G. Patel. M. L. Parmer et al have reported the partial molar volume of organic acids in binary aqueous solutions of urea at different temperature.

Volumetric studies have been carried out on nicotinic acid in water and in mixed aqueous solutions performed by Z. Orekhova et al. Guler Ayranci et al have measured the density and ultrasonic velocity of thiamine hydrochloride in aqueous solution of HCl/NaCl at different temperatures. I.V. Terekhova et al reported the volume studies the interactions between cyclodextrin and nicotinic acid in aqueous solutions. Hydration behaviour of nucleic bases in aqueous solution have been studied by V.A. Buckin. Density and speed of sound of the acid bases, nucleosides and nucleotides from aqueous to sodium and calcium chloride solution at different temperatures have been studied by N. Kishore and J. C. Ahluwalia.

P. S. Amutha et al have reported apparent molal volumes and partial molar volumes of aqueous solutions of some biologically important compounds at different temperature. Abhijit Sarkar et al have studied the thermodynamics of aqueous Nicotinic acid solutions in the presence of tetrabutylammonium hydrogen sulphate. Ishani Banik and Mahendra Nath Roy have reported the structural effects of three carbohydrates in nicotinic acid/water mixed solvents. Ravi Sharma et al have reported partial molar volume, viscometric properties of Nicotinic Acid in Binary Aqueous Mixtures of D-Lactose.

3. Objectives of research / Proposed hypothesis

Objective of the present work as below:

1. To examine thermodynamic properties of important nucleic acid bases, nucleosides and nucleotides etc in aqueous cosolute solution in order to understand the overall structure of nucleic acid bases, nucleosides and nucleotides etc in solution and structural fittings in solution.
2. To understand the solute-solute and solute-solvent interactions and overall behavior of the water soluble nucleic acid bases, nucleosides and nucleotides etc molecule in different cosolute solution.
3. To produce the valuable data of performed properties such as ultrasound velocity, density, refractive index and their derived thermodynamic properties such as volumetric, acoustical and optical properties etc. for the studied water soluble nucleic acid bases, nucleosides and nucleotides etc molecule in different cosolute solution.
4. To evaluate thermodynamic properties of nucleic acid bases, nucleosides and nucleotides etc which is depend upon concentration, temperature and relative composition of different cosolute solution.
5. To give comparative account of the thermodynamic behavior of different studied nucleic acid bases, nucleosides and nucleotides etc.

4. Methodology to be adopted

Following experimental methods will be used in present study.

1. For measurements of the density of the various solutions, the standard pycnometer of fixed volumes will be used.
2. Ultrasonic velocity measurements of the solutions will be carried out using ultrasonic interferometer with temperature maintained water bath.
3. Refractive indices of the solutions will be carried out by using Abbes refractometer at constant temperature.

5. Importance of study/Society application

(International status, national status & Significance of study)

The molecular interactions of nucleic acid bases, nucleosides and nucleotides with the different chemical compound such as salt, sugar, amino acids, vitamins and biologically important drugs in aqueous solution is a significant factor for maintaining the structural

behavior of nucleic acid bases, nucleosides and nucleotides. Consequently, the characterization of thermo-physical properties of solute solvation can give a hand in understanding the stability of nucleic acid bases, nucleosides and nucleotides. Interaction of nucleic acid bases, nucleosides and nucleotides with salt, sugar, amino acids and biologically important drugs in aqueous solution have been used widely in food, drug and pharmaceutical industries.

- **International status**

Over the last three decades, the revolutionary development in thermodynamic parameters or properties in aqueous solution have done. The researcher gives the great contribution in the investigation of physicochemical, thermodynamic properties of nucleic acid bases, nucleosides and nucleotides and biologically important compounds throughout the International level.

1. A.F. Fucaloro, K. Dewey, G. Fan, K. Imuta, D. Jensen and M. Muranaka. Joint Science Department, Mills Ave., Claremont, USA. This group worked on the thermodynamic properties of nucleic acid bases and bioactive molecules.
2. Z. Orekhova , E. Manzurola , M Ben-Ham , A. Apelblat. Department of Research and Development, Negev Academic College of Engineering and Department of Chemical Engineering, Ben Gurion University of the Negev, Beer Sheva, Israel. This team performed the density, ultrasonic velocity and optical properties of bio-organic acids and vitamins in aqueous solution.
3. Irina V. Terekhova, Rosario De Lisi, G. Lazzara, Stefania Milioto and Nicola Muratore Institute of Solution Chemistry of Russian Academy of Sciences and Dipartimento di Chimica Fisica F. Accascina', Universit degli Studi di Palermo, Viale delle Scienze, Parco D'Orleans Palermo, Italy. This research group worked on thermophysical properties of cyclodextrins and nicotinic acid in aqueous media.
4. Wojciech Zielenkiewicz, Anna Zielenkiewicz, Jean-Pierre E. Grolier, Alain H. Roux and Genevieve Roux-Desgranges. Institute of Physical Chemistry of the Polish Academy of Sciences, Warszawa, Kasprzaka, Poland and Laboratoire de Thermodynamique et Cinetique and Chimique, URA, University Blaise Pascal, France. This research group worked on thermodynamic properties of alkylated derivatives of uracil and adenine in aqueous solution.

5. P. Szterner, Institute of Physical Chemistry of the Polish Academy of Sciences, Kasprzaka, Warsaw, Poland have been studied the thermodynamic study of halogenated derivatives of nucleic acid bases at different temperatures.

The latest international researchers those have contributed for the thermodynamic properties of nucleic acid bases, nucleosides and nucleotides biological important compound in solution given below:

Cieplak, P., Kollman, P.A., Kabelac, M., Hobza, P., Schweizer, M. P., Broom, A. D., T'so, P.O.P., Hollis, D.P., Nakano, N.I., Igarashi, S.J., Fucaloro, A.F., Zanella, A., Widjaja, S., Widjaja, J., Lee, A., Chalikian, T.V., Cantor, C.R., Schimmel, P.R., A. Zielenkiewicz, G. Roux-Desgranges)A. H. Roux) J.-P. E. Grolier, K. L. Wierzchowski, and W. Zielenkiewicz.

- **National status**

Apart from the international contribution some of the national researchers have also made their mark contribution on thermodynamic properties of nucleic acid bases, nucleosides and nucleotides and bioactive compound in different aqueous media.

1. Tarlok S. Banipal, Harpreet Singh, Parampaul K. Banipal, Vickramjeet Singh. Department of Chemistry, Guru Nanak Dev University, Amritsar Punjab, India. This team worked on volumetric studies on nucleic acid bases and nucleosides in water.
2. Kalipada Sarkar 1 and Mahendra Nath Roy 2. 1 Islampur College, Islampur, Uttar Dinajpur, West Bengal, India. 2 Department of Chemistry, University of North Bengal, Darjeeling, West Bengal, India. This team worked on physicochemical properties of vitamins in aqueous media of ionic liquids, molecular interactions of nicotinic acid prevailing in salicylic acid + H_2O anthranilic acid + H_2O and o-nitrobenzoic acid + H_2O mixed system.
3. Ravi Sharma, Sonika and R.C.Thakur. Department of Chemistry, School of Chemical Engineering and Physical Sciences, Lovely Professional University, Phagwara, Punjab, India. This team worked on thermodynamic, acoustic behavior, partial molar volume of Nicotinic acid in binary aqueous mixtures of d-lactose.
4. M.L.Parmer, O.P. Sharma and M.K. Guleria. Department of Chemistry, Himachal Pradesh University, Summer Hill Station, Shimla, India. This team worked on partial molar volume of organic acids in binary aqueous solutions of urea.

5. P. Sahaya Amutha and X. Rosario Rajkumar. Department of Chemistry, Holy Cross College, Tiruchirappalli, India. This team worked on Apparent Molal Volumes and Partial Molar Volumes of Aqueous Solutions of Some Biologically Important Compounds.

Moreover, the latest national researchers those have contributed for the thermodynamic properties of DNA and RNA nucleic acid base and other biomolecules in different aqueous media.

A. Kundu, N. Kishore, S.G. Patel, T.S. Banipal, D. Kaur, G. Singh, B.S. Lark, P.K. Banipal Aminabhavi T. M., Sastry N. V., Patel, M. C. Kumar, S., Kusakabe K., Chanda R., Mrityunjaya, I. A., A. B. Sinha, R. Dey, M. Mizuguchi, M. Sakurai, K. Nitta, Abhijit Sarkar, Bijan Kumar Pandit, Biswajit Sinha, M.J. Iqbal, Q.M. Malik, R. Mehera, P. Yadav, D. Brahman, B. Sinha, M.L. Parmar, D.S. Banyal. These researchers focused on the various physicochemical, thermo-physical and thermodynamic properties of important biomolecule in aqueous as well as mixed solutions.

6. Significance of the study

To understand the molecular interaction of water soluble nucleic acid bases, nucleosides and nucleotides in aqueous solution of different cosolute such as sugars, electrolyte, non electrolyte, biological and pharmaceutical important drug by means of the systematic measurements of ultrasonic velocity, densities and refractive index. On the basis of these thermodynamic properties we obtain the data about interactions of important biomolecules such as nucleic acid bases/nucleosides/salt/amino acids/urea/drug. Investigation on the thermodynamic properties to provide significance information that ultimately leads to better understanding of solution behavior of water soluble vitamins. The structure promoting and breaking tendency of added nucleic acid bases and nucleosides for solvent and aqueous cosolute solutions is analyze through thermodynamic properties.

7. Proposed work Plan/Formulation and structure of Study:

The experimental work will be carried out as mentioned below:

Ist Year: Review of literature, calibrations and standardization of instrument etc. and study of density, ultrasonic velocity and refractive index and derived properties volumetric, acoustical and optical properties of water including other pure solvents will be carried out. The thermophysical properties of aqueous solutions of selected water soluble nucleic acid bases will be studied.

IInd Year: Study of the density, ultrasonic velocity and refractive index and derived properties such as volumetric, acoustical and optical properties of some water soluble nucleic acid bases and nucleosides at different temperature will be carried out in order to understand molecular interaction of nucleic acid bases, nucleosides in aqueous and aqueous cosolute (any two to three out of salt, urea, amino acids, sugars, drug) solution at different temperature through thermodynamic properties. Calculation of derived properties and data fitting to standard equation will be carried out. Communication of the results for publication.

IIIrd YEAR: Fitting the experimental data to different mathematical equations and scientific generalizations so as to get the calculated properties for studied system. The obtained result are interpreted and communication in referred journals.

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